Renewable Energy xxx (2017) 1–6

Contents lists available at ScienceDirect

Renewable Energy

journal homepage: www.elsevier.com/locate/renene

Modelling and development of a generator for a domestic gas-fired carbon-ammonia adsorption heat pump

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A R T I C L E I N F O

Article history:
Received 1 May 2016
Received in revised form
18 March 2017
Accepted 28 March 2017
Available online xxx

Keywords:
Carbon
Ammonia
Heat pump
Optimisation
Sorption

A B S T R A C T

Current development of ammonia-carbon gas fired heat pumps at the University of Warwick uses shell and tube adsorption generators with over 1700 water tubes of 1.2 mm outer diameter on a 3 mm pitch filled with vibrated carbon grains and powder. This geometry is not optimised and a dynamic simulation program has been written to determine how far from optimal the design is and also whether an alternative design of finned tubes offer advantages.

Three alternative carbon composites that use Expanded Natural Graphite (ENG), silane and lignin binders have been developed and tested to characterise their thermophysical properties so that they can be included in the simulations in order to improve the thermal transfer in the generators.

Results presented show that the shell and tube geometry is close to optimal and that the best performing material is the lignin+carbon composite.

Other type of geometry, a finned tube design, was modelled as it might offer improvements in performance and help reduce the complexity and cost of the manufacturing technique. Results show that for the same tube radius, the finned tube generator needs 7 times fewer tubes in order to achieve similar performances.

1. Introduction

Previous research at the University of Warwick has utilised shell and tube adsorption generators in heat pump prototypes in which water in 1.2 mm diameter tubes heats or cools granular carbon adsorbent surrounding the tubes which are on a 3 mm triangular pitch as shown in Fig. 1 [2].

The dimensions are thought to be reasonable values but are not optimised. Optimisation of materials or components for adsorption heat pumps is a complex task. For example, improving sorbent conductivity can reduce capital costs and physical size but reduce energy efficiency due to increased thermal mass. Enhancing conductivity of the adsorbent to an extreme level can result in either the water (tube side) heat transfer or tube-adsorbent thermal resistance becoming critical. Also, whatever the physical design of a machine, there is a trade-off of achievable power against efficiency that requires sophisticated control to minimise energy use whilst maintaining required comfort levels.

Two Matlab™ simulation models have been written to explore how varying dimensions, control parameters and adsorbent thermal properties affect the Coefficient of Performance (COP) and power output under specified conditions.

One model keeps the simple shell and tube geometry. This is a costly design to manufacture but has been proved with comparatively low conductivity carbon and high contact resistance.

One possibility of improving the heat transfer in the generator is the use of expanded natural graphite (ENG) as a matrix which has been widely utilised in the development of new types of adsorbents for adsorption refrigeration and air conditioning and heat pumping processes. The thermal conductivity of pure ENG is approximately 8 W/(mK) at a density of 1250 kg/m^3 [4]. ENG has been used as an additive for granular active carbon, in which the mixture thermal conductivity is improved by over 20 times [5]. Special attention must be paid when using compressed ENG matrices as the thermal conductivity of the mixture is highly anisotropic [10] and also increase the thermal mass of the generators.

Other possibility is the use of binders, either chemical or organic, that improve the bulk conductivity of the carbon. Examples of these binder can be vulcanised silicon rubber that increases the thermal conductivity of the granular carbon up to 1.3 W/(mK)

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http://dx.doi.org/10.1016/j.renene.2017.03.089

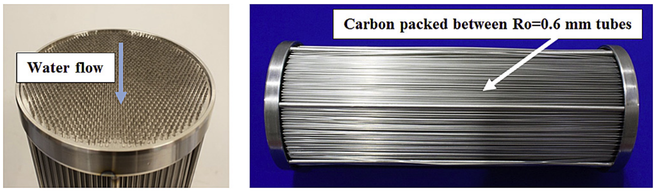

Fig. 1. Shell and (micro) tube sorption generator.

[3] or lignin binder that increases it from around 0.1 W/(mK) up to 0.44 W/(mK) [9].

This 2-D model simulates the heat transfer from water in a single tube to its surrounding unit cell of carbon throughout several thermodynamic cycles until the dynamics stabilise and the heating power per unit volume and COP are calculated.

The second model is based on the previous shell and tube model but it also includes the beneficial heat transfer effect of adding aluminium fins to the tubes as it was reported by Refs. [7] and [11].

Many parameters such as tube pitch, tube radius, tube wall thickness and fin and carbon thickness need to be varied in the simulation and there is of course no 'best' design and the optimum for highest power per unit volume is not the same as that for highest COP, but the trends can be explored and useful designs evaluated.

In order to avoid complicating the modelling task and optimisation a simple two bed cycle with heat recovery and no mass recovery was used. The only two control parameters were time for external heating/cooling to a constant temperature source/sink and the time for heat recovery.

2. Heat pump description

The heat pump that is currently under development at the University of Warwick is intended to be used in a domestic environment (space heating), replacing a gas condensing boiler. For space heating of a typical family home in the UK, a three bedroom semi-detached house, which is required to be maintained at an internal temperature of 18 °C, the heat pump should supply a heating power of 7 kW [6]. The 2-bed machine would be driven by the heat supplied by a gas burner and would use pressurised water as heat transfer fluid. The water used in the heating system of the house is passed through the ammonia condenser and then through the cooler (fluid to fluid heat exchanger) where it increases its temperature.

2.1. Generators design and sorption material

The type of heat exchanger used in this project is the previously mentioned shell and tube. The core of the generators was made of stainless steel 304 and the tubes have an outer diameter of 1.2 mm and an inner diameter of 0.8 mm. The end plates of the generators have a diameter of 144.5 mm and 1777 tubes were nickel brazed creating the core of the generator as seen in Fig. 1. After the core was filled with the carbon, it was slid inside the two halves of the generator shell. Finally, two flanges were attached at the ends of the shell completing the generator assembly.

The generator is effectively a thermally driven compressor and is the most critical part of the design.

The sorption material used in the generators is active carbon type 208C, especially good for heat pumping applications, based on coconut shell precursor manufactured by Chemviron Carbon Ltd.

In the heat exchanger, 3 kg of a mixture of 2/3 grains and 1/3 powder of carbon was vibrated reaching a bulk density of 650 kg/m^3 and yielded a thermal conductivity of 0.1 W/(mK) [8].

2.2. System description

The heat pump prototype was constructed to test the performance of the generators along with the carbon mixture and to validate the computational model developed of the machine. The water schematics and the ammonia pipework of the heat pump are shown in Fig. 2 a and b.

2.3. Experimental results and analysis

The machine was tested with a driving temperature of 150 °C and with an evaporating temperature of 5 °C. The machine was tested for two different delivery temperature cases:

- Underfloor heating: 36 °C flow delivery– 26 °C return.
- Low temperature radiators: 50 °C flow delivery– 40 °C return.

The results of the machine testing at the different delivery temperatures can be seen in Fig. 3a. Fig. 3b shows both the experimental and the simulated prediction of the heating powers of the condenser and cooler of the circled case in Fig. 3a. It is possible to observe that the experiment and the simulation are very similar.

Although the simulations and the experiments match, the performance of the system is low. In order to improve it, a better design of the generators along with a good choice of sorption material (carbon composite with enhanced thermal properties) is essential.

3. Materials

The adsorbents modelled include Chemviron 208C coconut shell loose carbon grains as well as other three different carbon composites that were developed by researchers of the University of Warwick with different binder materials in order to obtain a carbon composite with enhanced thermal properties than the ones of loose carbon grains.

3.1. Lignin binder

These lignin-carbon composites consist of blocks made of a mixture of carbon and ammonium salt of lignosulfonate, a lignin based binder. The composite is made by mixing carbon (grains, powder or a mixture of both), lignosulfonate and hot water (dissolves the binder and helps to create and homogenous mixture). The mixture is then compressed to the desired shape fired in an inert atmosphere in order to carbonise the organic binder.

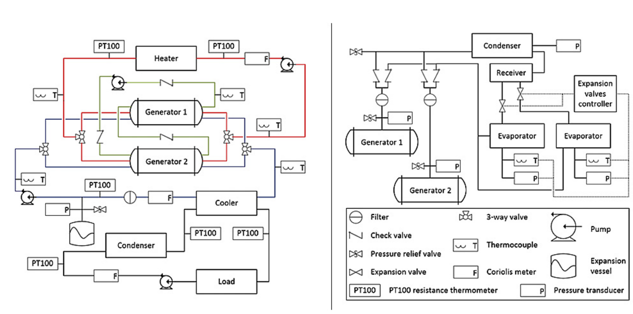

Fig. 2. a) Water and b) Ammonia pipework circuits.

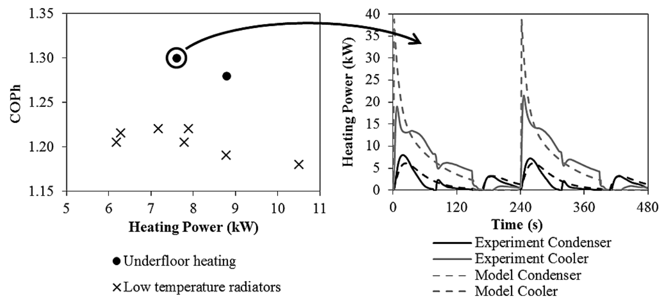

Fig. 3. a) COP vs Heating Power for underfloor heating and low temperature radiators (circled example case), b) Heating Power vs time of the circled underfloor heating case.

3.2. Silane binders

These silane-carbon composites blocks are made by mixing two aqueous solutions of different silanes. Then the carbon (grains, powder or a mixture of both) is added to the solution and after a process of evaporation of the excess solvent the mixture is compressed to the desired shape. Finally the samples are cured.

3.3. Expanded natural graphite (ENG)

These ENG-carbon composites consist of blocks made of a mixture of carbon and ENG flakes. The blocks of carbon and ENG are made by mixing between 50 and 25% weight of ENG and 50 and 75% respectively of carbon (grains, powder or a mixture of both). Then the mixture composite is compressed to the desired shape.

The thermophysical properties of the different carbon composites were measured in order to model their performance in the simulation.

The mass of refrigerant (ammonia) adsorbed in the beds over a cycle depends on the temperature and pressure of the system. The ammonia concentration is calculated with the modified Dubinin-Astakhov equation presented by Ref. [1].

$$x = x_0\, e^{-K\left({T}/{T_{sat}} - 1\right)^n} \ \mathrm{kg/kg} \qquad [1]$$

where T is the refrigerant/adsorbent temperature (K), T_{sat} is the saturation temperature (K), x is the adsorbed refrigerant concentration (kg/kg), x_0 is the maximum (limiting) concentration (kg/kg) and K and n are constants.

Since the adsorption characteristics of the carbon composites might vary due to the addition of the binders, adsorption tests were carried out with a Rubotherm magnetic suspension balance. Table 1 shows the Dubinin-Astakhov adsorption coefficients of the different carbons tested.

Apart from the sorption coefficients, Table 1 shows the density of the different sample materials used in the simulations and other thermal characteristics such as specific heat and thermal conductivity. The density of the ENG+carbon composites shown between brackets corresponds to the carbon density in the sample.

The specific heat of the carbon was calculated as a function of temperature and as the specific heats of the carbon and graphite are very similar, the same temperature dependent equation was used when simulating ENG + carbon composites.

The thermal conductivity of the samples was obtained with the Quickline-10 Anter machine.

4. Simulation models

The water-side heat transfer used in both models is laminar flow with a Nusselt number approximated to 4 and all other heat transfer is via conduction with the ability to include a steel-carbon resistance modelled by a thin layer of ammonia gas if required.

Typically a time step of 0.02 s was adequate to ensure that the solutions had converged and 4 full cycles were simulated to ensure that periodicity had been achieved. A range of equal heating and cooling times were modelled in combination with a range of heat recovery times so that an envelope of COPs and Specific Heating Powers (SHP, mean heat output in W/unit volume of generator) could be obtained.

Within the program, during the nominal isosteric heating and cooling the pressure at a new time step was derived iteratively with the constraint that the total mass of adsorbate within the generator was constant and during evaporation and condensation the pressure was maintained constant and mass change calculated.

4.1. Shell and tube design

The program is written as a two dimensional finite difference model in Matlab™. The unit cell is a hexagonal section as shown in Fig. 4a. The true outer surface in a shell and tube configuration would be a hexagonal adiabatic boundary but the approximation is made to a cylindrical boundary of the same contained volume.

The lengthwise cell is split into nl axial sections allowing the modelling of thermal waves if required and the carbon is split into nc equal radial sections. In the results presented, $nc = 3$ has proved adequate when compared with finer subdivisions. The pressurised water used to heat or cool and steel have only one radial element, but the water can be subdivided into multiple numbers of axial elements if the mass flow rate specified is so high that an element of water could flow past more than one axial element of steel in one time step.

The input parameters are the carbon bulk conductivity, specific heat, density and contact resistance, plus the water tube diameter,

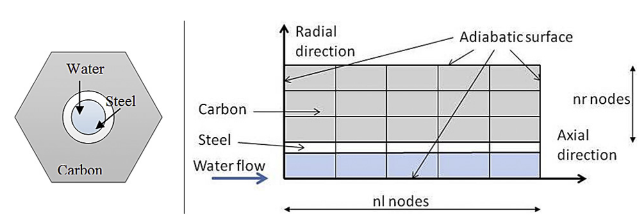

Fig. 4. a) Shell and tube cross section area of unit cell, b) Longitudinal unit cell.

Table 1
Adsorbent properties.

Adsorbent	Density (kg/m^3)	Specific heat (J/(kg K))	Thermal conductivity (W/(m K))	x_0	n	K
Granular 208C	650	175+2.245*T(K)	0.10	0.2775	5.445	1.460
208C + lignin binder	791	175+2.245*T(K)	0.32	0.2568	4.666	1.297
208C + silane binder	704	175+2.245*T(K)	0.26	0.2344	4.453	1.318
75% 208C + 25% ENG	770 (578)	175+2.245*T(K)	1.03	0.2775*0.75	5.445	1.460
50% 208C + 50% ENG	1025 (513)	175+2.245*T(K)	1.65	0.2775*0.5	5.445	1.460

wall thickness and pitch.

4.2. Finned tube design

Whilst the shell and tube designs have been demonstrated and in principle have some advantages, the difficulty of manufacturing them at reasonable cost has prompted a re-examination of other geometries, including the use of aluminium fins on tubes within a shell, thereby reducing the number of tubes. In this work the unit cell has been modelled as in Fig. 5.

In order to keep the simulation stable whilst the heat transfer in the metallic segments was modelled and while keeping the total computation time reasonable, at a time step roughly 0.05 times that of the carbon was used for all the metallic elements.

The geometry parameters that can be varied in this model are the inner and outer tube diameter and the tube pitch in addition to the fin thickness and the carbon thickness between fins.

5. Simulation results

In all the simulations run, in order to compare designs, the cooling phase assumes an inlet water temperature of 50 °C, in the heating phase the water inlet is at 170 °C, the evaporating temperature is 5 °C and the condensing at 50 °C.

The heating/cooling cycle times and recovery times used in the simulations vary between 20 and 200 s and between 0 and 50 s respectively.

5.1. Shell and tube

First of all, the current generator geometry (outer radius 0.6 mm and pitch 3 mm) was simulated for all the candidate materials previously presented. Fig. 6 shows the simulation results obtained and indicates the performance envelope for each material.

It can be observed that the performance envelopes of the carbon composites made with 25 and 50% ENG are quite flat due to the high thermal conductivities of the samples (1 and 1.65 W/(mK) respectively) because they desorb and adsorb ammonia quickly meaning short cycle times (70 s). Also, because their carbon density is low, 513 and 578 kg/m^3, their heating COP's at low powers remain relatively lower than the rest of the samples reaching 1.235 and 1.27.

The vibrated grains sample shows the steepest envelope due to its low thermal conductivity. It reaches the highest COP, 1.29, because it is the sample that more ammonia can adsorb and desorb during a cycle (highest x_0 value) but it needs very long cycle times (460s) to achieve this and the output power falls to less than 1000 kW/m^3.

The silane-carbon composite needs relatively long cycle times of 160 s to obtain a reasonable COP of 1.26 with a reasonable output power of 1150 kW/m^3. The lignin-carbon composite shows a good performance obtaining a COP of 1.28 at a reasonable output power (1150 kW/m^3) with a cycle time of 100 s.

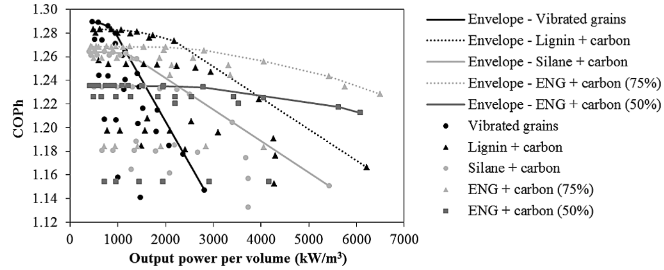

Fig. 6. COP v. Output power for all adsorbents, 0.6 mm tube radius and 3 mm pitch.

Due to the good performance shown by the lignin-binder composite, it was used to model other geometry cases in order to obtain an optimised generator.

Fig. 7 shows the performance envelopes of different tube pitch generators for the 0.6 mm tube radius and lignin+carbon composite. The heating/cooling and recovery times are indicated for every case.

Pitches 4 and 3.5 mm show higher COP at output powers lower than 1000 kW/m^3 but at higher output powers the COP drops significantly. The other cases, 2.8, 3 and 3.2 mm show good output power/COP relationships.

In order to make the generator easier to manufacture, the possibility of bigger tubes was explored. Fig. 8 shows the results obtained when modelling a tube radius of 1.5 mm and three different pitches and it is compared to the 0.6 mm outer radius tube. It can be observed that with a bigger tube the COP achieved by the system is lower.

Fig. 9 illustrates the detailed results obtained for the lignin+carbon composite with a 0.6 mm tube outside radius (0.4 mm internal radius) and 3 mm tube pitch, as per the current design. It shows how for a range of heating/cooling and heat recovery times the combinations of COP and output power vary.

It can be observed that heat recovery significantly increases the COP. For this material and geometry case, recovery time of 30 s and heating/cooling time of 50 s (cycle time of 160 s) is a good combination in order to obtain a good machine performance.

Given that the present design of generator at Warwick is not far from the optimum for a shell and tube design and that they all present challenges in reliable cost effective manufacture, the finned tube is worth exploring.

5.2. Finned tube results

All the simulations presented in this section were run with the lignin+carbon composite as it performs superiorly to the other

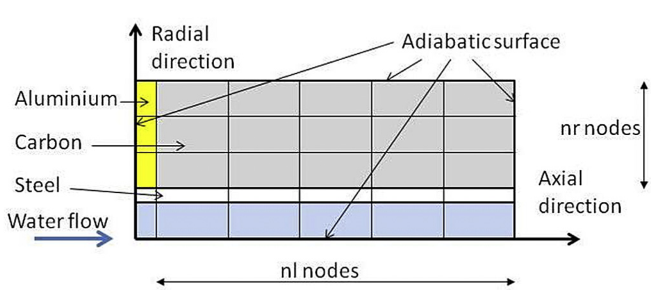

Fig. 5. Finned tube unit cell.

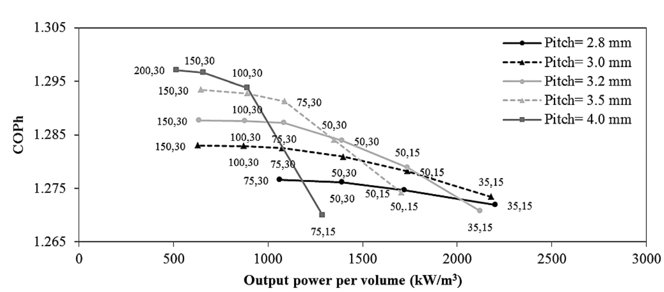

Fig. 7. COP v. Output power for lignin+carbon composite with a 0.6 mm radius tube and a range of tube pitch.

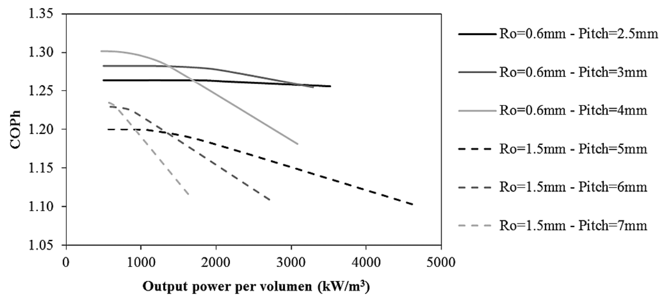

Fig. 8. COP v. Output power for different outer radii and pitch tube for the lignin+carbon composite.

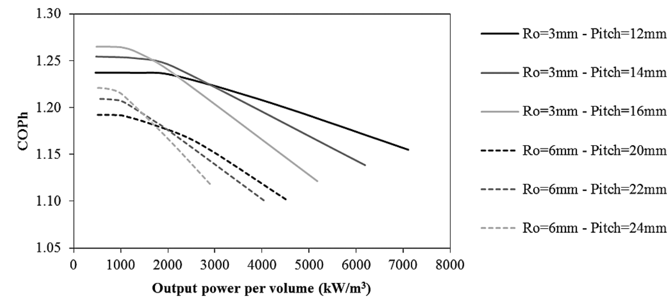

Fig. 11. COP v. Output power for different outer radii and pitch tube for the lignin+carbon composite.

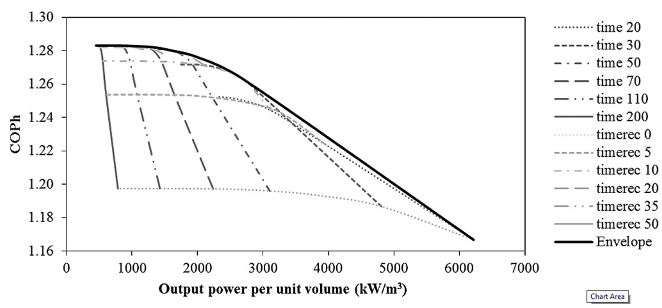

Fig. 9. COP v. Output power for carbon+lignin composite, 0.6 mm radius tube and 3 mm pitch for different heating/cooling and recovery times.

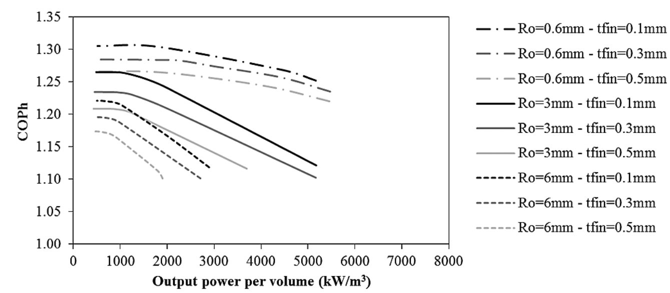

Fig. 12. COP v. Output power for different outer radii tube and fin thickness for the lignin+carbon composite.

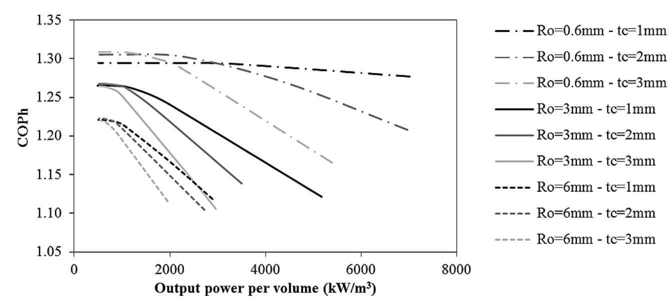

Fig. 13. COP v. Output power for different outer radii and carbon thickness for the lignin+carbon composite.

composites.

One early trend observed was that as tube radii and pitches grew (desirable in terms of manufacturing) the water side heat transfer became limiting and the largest thermal resistance was between water and steel. Since techniques to improve surface area and/or heat transfer coefficient exist, the model simply augmented the W/K of a length of tube by a factor of 10 in order to explore what the potential is on the adsorbent side. This is illustrated in Fig. 10 which shows how COP and SHP vary with cycle times for both augmented and unaugmented water side heat transfer (h_w).

Fig. 11 shows the performance envelopes of two different tube radii, 3 and 6 mm and three different tube pitches for each case. The fin thickness used in all the simulations corresponds to 0.1 mm and the carbon thickness corresponds to 1 mm.

It can be observed that the smallest tube, 3 mm outer radius, achieves the highest COP's.

Fig. 12 shows the performance envelopes of three different tube radii, 0.6, 3 and 6 mm and three different fin thicknesses for each case. The carbon thickness in the Ro = 0.6 mm corresponds to 2 mm whilst in the other cases corresponds to 1 mm. The pitches in the 0.6, 3 and 6 mm outer radii cases correspond to 6, 16 and 24 mm.

Fig. 13 shows the performance envelopes of three different tube radii, 0.6, 3 and 6 mm and three different carbon thicknesses for each case. The fin thickness used in all the simulations corresponds to 0.1 mm and the pitches in the 0.6, 3 and 6 mm outer radii cases

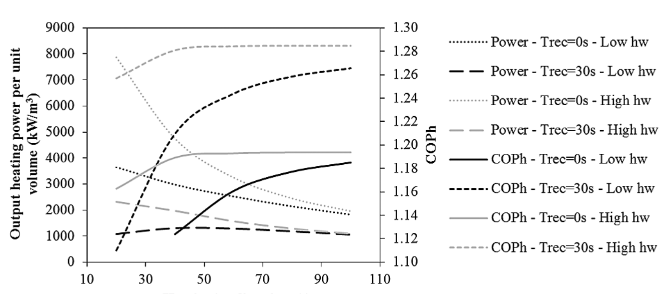

Fig. 10. COP and SHP for lignin+carbon composite with a range of control times with low and high water side heat transfer.

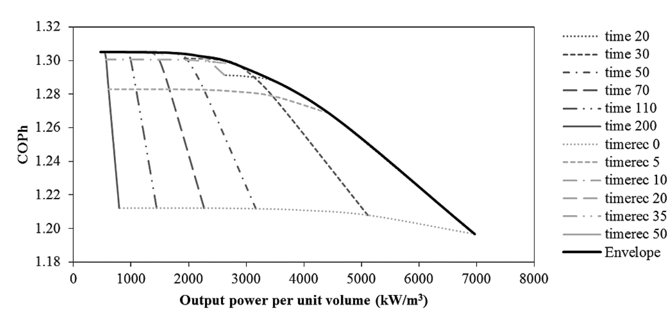

Fig. 14. COP v. Output power for carbon+lignin composite, 0.6 mm radius tube, 0.1 mm fin thickness, 2 mm carbon thickness and 6 mm pitch for different heating/cooling and recovery times.

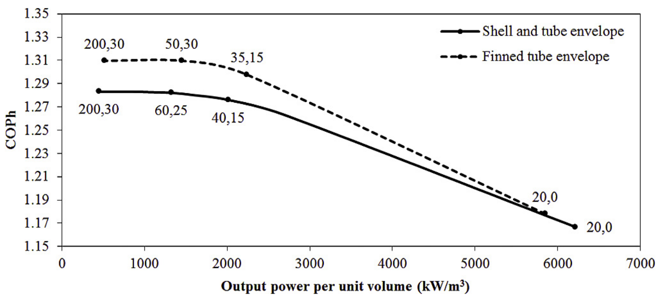

Fig. 15. COP v. Output power comparison of shell and tube and finned tube generators with carbon+lignin composite.

correspond to 6, 16 and 24 mm.

Fig. 14 illustrates the detailed results obtained for the lignin+carbon composite with a 0.6 mm tube outside radius (0.4 mm internal radius) and 6 mm tube pitch s this case shows a good performance envelope.

The figure shows how for a range of heating/cooling and heat recovery times the combinations of COP and output power vary.

It can be observed that heat recovery significantly increases the COP. For this material and geometry case, recovery time of 30 s and heating/cooling time of 50 s (cycle time of 160 s) is a good combination in order to obtain a good machine performance.

5.3. Geometries comparison

The envelopes of the best case of shell and tube, Fig. 9, and a case of finned tube have been plotted together in Fig. 15 for comparison along with its heating/cooling and recovery times.

The tube in both examples has an outer radius of 0.6 mm and an inner radius of 0.4 mm and the sorption material modelled is the same, lignin-carbon composite. In the case of the finned tube the fin thickness is 0.1 mm and the carbon thickness between fins is 2 mm.

In the shell and tube case, the tube pitch is 3 mm whilst in the finned tube case, the tube pitch is 8 mm.

Both cases show similar performance, having the finned tube case slightly higher COP but the interesting thing to highlight is that due to the difference in tube pitches, the finned tube generator would need 7 times fewer tubes than the shell and tube one in order to obtain similar performance which would reduce their manufacturing cost.

6. Conclusions

The carbon composite materials developed and characterised were modelled in a shell and tube geometry but only one of them, lignin+carbon, shows good performance. The ENG+carbon composites do not reach an acceptable COP due to their low carbon density, the vibrated grains carbon do not deliver enough heating power and the silane+carbon composite does not reach a good COP and power output due to its low adsorption/desorption rate and due to its low thermal conductivity.

The existing shell and tube design (inner and outer radii 0.4 and 0.6 mm respectively, tube pitch 3 mm) modelled with the lignin+binder composite is close to the optimum but with an inherent cost and reliability challenges. Typical cycle times for this geometry and material would be between 100 and 160 s.

For the shell and tube case the smaller the tube the higher the COP and the output power when paired with an according tube pitch but this would contribute to the costly manufacturing process of the heat exchanger and would increase the water pressure drop.

It was observed that as the tube radii and pitches in the finned tube case increased in size the water side heat transfer became limiting and the largest thermal resistance was between water and steel. The model augmented the W/K of the tube by a factor of 10 and techniques to improve surface area and/or heat transfer coefficient in the tubes will be investigated.

In the case of the finned tube geometry, smaller tubes yield higher COP but their tube pitches are double or triple the ones corresponding to the shell and tube case. Given that the number of tubes needed varies inversely with the square of the pitch, this is a significant advantage.

For the different tube sizes modelled in with the finned tube geometry a fin thickness of 0.1 mm was found to be optimal. Regarding the carbon thickness between fins, for the tube radii of 3 and 6 mm the optimal was found to be 1 mm whilst in the case of an outer radius of 0.6 mm the optimum corresponds to a thickness of 2 mm. Typical cycle times for this geometry and material would be between 100 and 160 s.

Due to the higher tube pitches and bigger tube diameters in the finned tube designs it is possible they could be significantly lower in production cost as 7 times fewer tubes are needed to offer a similar performance.

For both geometries a recovery time of around 30 s and heating/cooling time of between 50 s (cycle time of 170 s) is a good combination in order to obtain a good machine performance.

Further work will be done to manufacture and test in a large temperature jump apparatus a preferred fin and tube design and then to test it before attempting to build a full sized generator for evaluation in a kW scale machine.

Acknowledgements

We would like to thank Chemviron Carbon for supplying the carbon and the organic binder used in the experiments, Fraunhofer ISE for carrying out the measurements with the LFA 467 HyperFlash machine and Lucio Bonaccorsi (Mediterranea University of Reggio Calabria) and Dorotea Spadaro (University of Warwick) for their help with the silane binder development.

This research was supported by the EPSRC grant to the University of Warwick (EP/K011847/1).

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Please cite this article in press as: A.M. Rivero-Pacho, et al., Modelling and development of a generator for a domestic gas-fired carbon-ammonia adsorption heat pump, Renewable Energy (2017), http://dx.doi.org/10.1016/j.renene.2017.03.089